

Elastic scattering of positrons by helium atoms

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Abstract : The differential and total cross sections for elastic scattering of positrons by helium atoms are computed in the energy range 100 to 1000 eV. In the present study Unitarised eikonal—Born series (UEBS) method is used. The comparison of present results with the other theoretical and experimental results shows that the present results are in better agreement with the experimental values

Keywords : Elastic scattering, positrons, helium atoms, differential and total cross sections.

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1. Introduction

The study of scattering of charged particles by helium atoms has been considered as an important process in astrophysics and plasma physics. Different approximations have been used in the study of the above process. In the present investigation unitarised eikonal-Born series method (Byron *et al* 1982) is used.

After eikonal approximation in potential scattering theory (Moliere 1947), Glauber (1959) extended it by using a frozen target approximation to convert many body scattering problem into a potential scattering problem in which the potential depends on the coordinates of the target. However original eikonal approximation could not be free from serious drawbacks (Byron *et al* 1973). So Byron and Joachain (1973b) made a detailed comparison between the terms of Born and eikonal series (in potential scattering) or the Born and Glauber series (for multiparticle collisions) and formulated the eikonal-Born series (EBS) method (Byron and Joachain 1973b). In this approach they made an attempt to eliminate the deficiencies of the eikonal approximation and the Glauber many-body generalisation within the framework of the perturbation theory.

On the other hand Wallace (1971, 1973) also proposed a systematic correction to the eikonal phase. But it was remarked (Byron *et al* 1981) that Wallace amplitude did not eliminate all the difficulties inherent in the Glauber amplitude because Wallace extension of the Glauber approximation did not account for long range polarisation effect at small angle

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and represented inadequate absorption effects in the same region. To eliminate above difficulties Byron *et al* (1982) suggested to remove the term of many-body Wallace amplitude which is of second order in the projectile target interaction and to replace it by the second Born term. The direct amplitude thus obtained was called unitarised eikonal-Born series (UEBS) amplitude which has all the strength of the EBS method at small and intermediate angles where perturbation theory is rapidly convergent but in addition at large angles where the small distance singularity of central coulomb potential is important. It gives satisfactory results due to two leading terms (in power of k_i^{-1}) of each order of perturbation theory summed up to all orders.

2. Theory and calculations

According to UEBS method (Byron *et al* 1982) scattering amplitude is given by

$$f_{UEBS} = f_W - \bar{f}_{W2} + \bar{f}_{B2} \quad (1)$$

where many-body Wallace amplitude f_W is given by

$$f_W = \frac{k_i}{2\pi i} \int \exp(i \Delta \cdot b)$$

$$\left\langle \Psi_m(x) \left| \left[\exp i \left\{ k_i^{-1} \chi_0(b, x) + k_i^{-3} \chi_1(b, x) \right\} - 1 \right] \right| \Psi_0(x) \right\rangle d^2b \quad (2)$$

For ($S \rightarrow S$) transition equation (2) can be written as

$$f_W(S \rightarrow S) = -iki \int_0^\infty J_0(\Delta b)$$

$$\left\langle \Psi_m(x) \left| \left[\exp i \left\{ k_i^{-1} \chi_0(b, x) + k_i^{-3} \chi_1(b, x) \right\} - 1 \right] \right| \Psi_0(x) \right\rangle b db \quad (3)$$

The second order Wallace term \bar{f}_{W2} is given by

$$\bar{f}_{W2} = (2\pi)^{-1} \int \exp(i \Delta \cdot b)$$

$$\left\langle \Psi_m(x) \left| \frac{1}{2} i k_i^{-1} \chi_0(b, x) + k_i^{-2} \chi_1(b, x) \right| \Psi_0(x) \right\rangle d^2b \quad (4)$$

For ($S \rightarrow S$) transition real and imaginary part of \bar{f}_{W2} can be written as

$$Re \bar{f}_{W2}(S \rightarrow S) = k_i^{-2} \int_0^\infty J_0(\Delta b) \left\langle \Psi_m(x) \left| \chi_1(b, x) \right| \Psi_0(x) \right\rangle b db \quad (5)$$

$$\text{Im } \bar{f}_{w2}(S \rightarrow S) = \frac{1}{2} k_i^{-1} \int_0^\infty J_0(\Delta b) \left\langle \Psi_m(x) \chi_0^2(b_1 x) \Psi_0(x) \right\rangle b db \quad (6)$$

where

$$\chi_0(b, x) = - \int_{-\infty}^{\infty} V(b, z, x) dz \quad (7)$$

$$\chi_1(b, x) = \frac{1}{2} \int_{-\infty}^{\infty} (\nabla \chi_+ \cdot \nabla \chi_-) dz \quad (8)$$

With

$$\chi_+(b, z, x) = - \int_{-\infty}^z V(b, z', x) dz' \quad (9)$$

$$\chi_-(b, z, x) = - \int_z^{\infty} V(b, z', x) dz' \quad (10)$$

Simplified second Born term is given by (Joachain 1979)

$$\bar{f}_{\beta 2} = \frac{2}{\pi^2} \int dK \frac{1}{K^2 - K'^2 - i\epsilon K_i^2 K_f^2} \left\langle 0 \left| \left[\exp(-i k_f \cdot r) - 1 \right] \left[\exp(-i k_i \cdot r) - 1 \right] \right| 0 \right\rangle \quad (11)$$

with $K_i = k_i - K$, $K_f = k_f - K$, $K'^2 = K^2 - 2\bar{\omega}$

where $\bar{\omega}$ = average excitation energy

In the present calculations for $e^+ - \text{He}$ collision, the model as shown in Figure 1 is used.

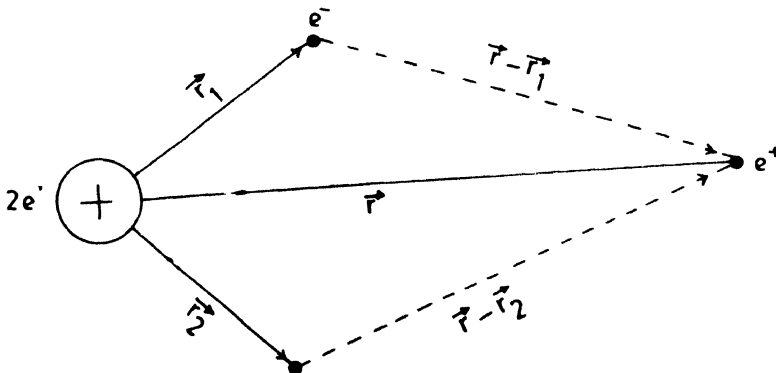


Figure 1. A model representation for elastic scattering of positrons by helium atoms.

$$\text{Potential } V \text{ (in atomic unit)} = \left[\frac{2}{r} - \frac{1}{|r - r_1|} - \frac{1}{|r - r_2|} \right] \quad (12)$$

According to cylindrical coordinates,

$$r = b + z\hat{k}, r_1 = b_1 + z_1\hat{k}, r_2 = b_2 + z_2\hat{k}$$

For $e^+ - \text{He}$ collision

$$\chi_0(b, x) = \ln \left[\left(\frac{|b - b_1|^2}{b^2} \right) \left(\frac{|b - b_2|^2}{b^2} \right) \right] \quad (13)$$

$$\chi_1(b, x) = 2I_1 + 2I_2 - I_3 \quad (14)$$

where

$$I_1 = \frac{\pi}{(b\beta_1)^{1/2}} \left[P_{-1/2}(U_1) - \hat{\beta}_1 \cdot \hat{\beta}_1 P_{1/2}(U_1) \right]$$

$$I_2 = \frac{\pi}{(b\beta_2)^{1/2}} \left[P_{-1/2}(U_2) - \hat{\beta}_2 \cdot \hat{\beta}_2 P_{1/2}(U_2) \right]$$

$$I_3 = \frac{\pi}{(\beta_1\beta_2)^{1/2}} \left[P_{-1/2}(U_3) - \hat{\beta}_1 \cdot \hat{\beta}_2 P_{1/2}(U_3) \right]$$

Where

$$U_1 = \frac{b^2 + \beta_1^2 + z_1^2}{2b\beta_1}$$

$$U_2 = \frac{b^2 + \beta_2^2 + z_2^2}{2b\beta_2}$$

with

$$U_3 = \frac{\beta_1^2 + \beta_2^2 + (z_2 - z_1)^2}{2\beta_1\beta_2}$$

$$\beta_1 = b - b_1, \beta_1 = |\beta_1|, \hat{\beta}_1 = \frac{\beta_1}{|\beta_1|}$$

$$\beta_2 = b - b_2, \beta_2 = |\beta_2|, \hat{\beta}_2 = \frac{\beta_2}{|\beta_2|}$$

$P_{1/2}$ and $P_{-1/2}$ are Legendre functions. In the above calculations tables of integrals and mathematical functions [Abramowitz and Stegun (1964), Gradshteyn and Ryzhik (1965)] were used. In the present calculations Hartree-Fock wave function for groundstate of helium atom is used. It is given by

$$\Psi_{1s}(r_1, r_2) = \frac{(Ae^{-ar_1} + Be^{-\beta r_1})(Ae^{-ar_2} + Be^{-\beta r_2})}{4\pi} \quad (15)$$

$$A = 2.60505, B = 2.08144, a = 1.41, \beta = 2.61$$

For $e^+ - \text{He}$ collision simplified second Born term is given by (Kusum Lata 1984).

$$\begin{aligned}
\bar{f}_{B2} = & \sum_{i=1}^3 \frac{16a_i N^2}{\lambda_i^3} \\
& \left[\frac{4K^2(K^2 + 2\lambda_i^2)}{(K^2 + \lambda_i^2)^2} A_p(0, 0) + 8A_p(\lambda_i, 0) - 8\lambda_i^2 \frac{\partial}{\partial \lambda_i^2} A_p(\lambda_i, 0) \right] \\
& - \sum_{i=1}^3 \sum_{j=1}^3 \frac{(8N^2)^2 8a_i a_j}{\lambda_i^3 \lambda_j^3} A_p(\lambda_i, \lambda_j) \\
& - \lambda_i^2 \frac{\partial}{\partial \lambda_i^2} A_p(\lambda_i, \lambda_j) - \lambda_j^2 \frac{\partial}{\partial \lambda_j^2} A_p(\lambda_i, \lambda_j) + \\
& \lambda_i^2 \lambda_j^2 \frac{\partial^2}{\partial \lambda_i^2 \partial \lambda_j^2} A_p(\lambda_i, \lambda_j) + \sum_{i=1}^3 \sum_{j=1}^3 \frac{(8N^2)^2 8a_i a_j}{\lambda_i^3 \lambda_j^3} \\
& \left[A_{k_i}(\lambda_i, \lambda_j) - \lambda_i^2 \frac{\partial}{\partial \lambda_i^2} A_{k_i}(\lambda_i, \lambda_j) \right. \\
& \left. - \lambda_j^2 \frac{\partial}{\partial \lambda_j^2} A_{k_i}(\lambda_i, \lambda_j) + \lambda_i^2 \lambda_j^2 \frac{\partial^2}{\partial \lambda_i^2 \partial \lambda_j^2} A_{k_i}(\lambda_i, \lambda_j) \right] \quad (16)
\end{aligned}$$

Where

$$\begin{aligned}
K &= 2k_i \sin \frac{\theta}{2} & \lambda_1 &= 2a & a_1 &= A^2 \\
P^2 &= k_i^2 - 2K & \lambda_2 &= 2\beta & a_2 &= B^2 \\
N &= \frac{1}{16\pi^{\frac{3}{2}}} & \lambda_3 &= a + \beta & a_3 &= 2AB
\end{aligned}$$

$$A_p(a, \beta) = \frac{1}{2(b^2 - a_c)^{\frac{1}{2}}} \ln \left[\frac{b + (b^2 - a_c)^{\frac{1}{2}}}{b - (b^2 - a_c)^{\frac{1}{2}}} \right]$$

$$b = ip [K^2 + (a + \beta)^2] + \beta(-P^2 - k_i^2 + a^2) + a(-P^2 + k_f^2 + \beta^2)$$

$$\begin{aligned}
a_c = & [K^2 + (a^2 + \beta^2)] \left[k_i^2 + a^2 - p^2 - 2iaP \right] \\
& \left[k_f^2 - P^2 + \beta^2 - 2i\beta P \right]
\end{aligned}$$

$$k_f = k_i - K$$

The differential cross section $I(\theta)$ for e^+ -He elastic collision is given by

$$I(\theta) = |f_{UEBS}|^2 \quad (17)$$

The total cross section Q_t for e^+ -He elastic collision is obtained from optical theorem as

$$Q_t = \left(\frac{4\pi}{k_i} \right) \text{Im} f_{UEBS}(\theta = 0) \quad (18)$$

Using above equations, the differential cross sections (DCS) and total cross sections (TCS) are calculated for elastic scattering of positron from ground state of helium atom for the incident positron energies 100 eV, 400 eV and 700 eV.

3. Results and discussion

The present results of total cross sections (TCS) at the energies 100 eV, 400 eV and 700 eV are given in the Table 1. The results of differential cross sections (DCS) at the energies 100 eV, 400 eV and 700 eV are presented in Tables 2, 3 and 4 respectively. The present TCS and DCS results are compared with the theoretical results of EBS method (Byron 1977b),

Table 1. The total cross sections (a^2) for the elastic scattering of positrons by helium atoms.

Energy	Das <i>et al</i> (1981)	Modified Das method (Kusum Lata 1984)	EBS	Present UEBS	Kauppila <i>et al</i> (1984)
100 eV	0.76	3.53	4.57	4.062	3.64
400 eV	0.82	1.60	1.71	1.659	1.64
700 eV	0.67	1.05	1.10	1.013	—

Table 2. The differential cross sections ($a^2 \text{Sr}^{-1}$) for the elastic scattering of positrons by helium atoms for energy 100 eV. The numbers in parentheses indicate powers of ten.

100 eV					
Energy (deg)	Das <i>et al</i> (1981)	Modified Das method (Kusum Lata 1984)	EBS	Present UEBS	
0	2.86 (−2)	6.27 (−1)	1.24	1.004	
5	5.24 (−2)	5.34 (−1)	1.01	8.288	
10	8.89 (−2)	4.33 (−1)	7.85 (−1)	6.175 (−1)	
20	1.44 (−1)	2.66 (−1)	4.34 (−1)	3.738 (−1)	
30	1.43 (−1)	1.58 (−1)	2.31 (−1)	1.817 (−1)	
40	1.12 (−1)	9.39 (−2)	1.33 (−1)	1.086 (−1)	
50	7.86 (−2)	5.72 (−2)	8.88 (−2)	7.898 (−2)	
60	5.30 (−2)	3.66 (−2)	7.05 (−2)	6.129 (−2)	
70	3.59 (−2)	2.49 (−2)	6.26 (−2)	5.104 (−2)	
80	2.51 (−2)	1.79 (−2)	5.88 (−2)	4.365 (−2)	
90	1.84 (−2)	1.36 (−2)	5.63 (−2)	3.758 (−2)	
100	1.41 (−2)	1.07 (−2)	5.43 (−2)	3.296 (−2)	
120	9.48 (−3)	7.43 (−3)	5.06 (−2)	2.719 (−2)	
140	7.39 (−3)	5.78 (−3)	4.77 (−2)	2.348 (−2)	
160	6.46 (−3)	4.98 (−3)	4.59 (−2)	2.081 (−2)	
180	6.19 (−3)	4.74 (−3)	4.52 (−2)	1.977 (−2)	

Table 3. The differential cross sections ($a_0^2 \text{Sr}^{-1}$) for the elastic scattering of positrons by helium atoms for energy 400 eV. The numbers in parentheses indicate powers of ten.

400 eV				
Energy (deg.)	Das <i>et al</i> (1981)	Modified Das method (Kusum Lata 1984)	EBS	Present UEBS
0	1.57 (-1)	5.31 (-1)	6.02 (-1)	5.633 (-1)
5	3.18 (-1)	5.64 (-1)	5.91 (-1)	5.083 (-1)
10	3.15 (-1)	4.14 (-1)	4.23 (-1)	3.912 (-1)
20	1.74 (-1)	1.83 (-1)	1.80 (-1)	1.687 (-1)
30	7.74 (-2)	7.73 (-2)	7.53 (-2)	7.054 (-2)
40	3.56 (-2)	3.54 (-2)	3.52 (-2)	3.432 (-2)
50	1.81 (-2)	1.81 (-2)	1.90 (-2)	1.801 (-2)
60	1.03 (-2)	1.03 (-2)	1.16 (-2)	1.078 (-2)
70	6.52 (-3)	6.31 (-3)	7.82 (-3)	6.849 (-3)
80	4.45 (-3)	4.16 (-3)	5.66 (-3)	4.836 (-3)
90	3.24 (-3)	2.91 (-3)	4.34 (-3)	3.577 (-3)
100	2.49 (-3)	2.14 (-3)	3.48 (-3)	2.790 (-3)
120	1.67 (-3)	1.33 (-3)	2.49 (-3)	1.790 (-3)
140	1.28 (-3)	9.61 (-4)	1.99 (-3)	1.402 (-3)
160	1.10 (-3)	7.96 (-4)	1.75 (-3)	1.108 (-3)
180	1.04 (-3)	7.48 (-4)	1.60 (-3)	1.095 (-3)

Table 4. The differential cross sections ($a_0^2 \text{Sr}^{-1}$) for the elastic scattering of positrons by helium atoms for energy 700 eV. The numbers in parentheses indicate powers of ten.

700 eV				
Energy (deg.)	Das <i>et al</i> (1981)	Modified Das method (Kusum Lata 1984)	EBS	Present UEBS
0	2.34 (-1)	5.24 (-1)	5.42 (-1)	5.102 (-1)
5	4.07 (-1)	5.39 (-1)	5.46 (-1)	4.308 (-1)
10	3.13 (-1)	3.52 (-1)	3.52 (-1)	3.391 (-1)
20	1.16 (-1)	1.19 (-1)	1.18 (-1)	1.117 (-1)
30	4.10 (-2)	4.16 (-2)	4.12 (-2)	4.078 (-2)
40	1.68 (-2)	1.70 (-2)	1.72 (-2)	1.669 (-2)
50	8.12 (-3)	8.10 (-3)	8.50 (-3)	8.313 (-3)
60	4.51 (-3)	4.37 (-3)	4.81 (-3)	4.599 (-3)
70	2.78 (-3)	2.60 (-3)	3.02 (-3)	2.812 (-3)
80	1.87 (-3)	1.67 (-3)	2.05 (-3)	1.915 (-3)
90	1.34 (-3)	1.15 (-3)	1.49 (-3)	1.374 (-3)
100	1.01 (-3)	8.40 (-4)	1.14 (-3)	1.091 (-3)
120	6.64 (-4)	5.16 (-4)	7.66 (-4)	6.703 (-4)
140	5.00 (-4)	3.70 (-4)	5.83 (-4)	5.157 (-4)
160	4.25 (-4)	3.05 (-4)	4.99 (-4)	4.399 (-4)
180	4.04 (-4)	2.88 (-4)	4.78 (-4)	4.112 (-4)

The differential cross section $I(\theta)$ for e^+ -He elastic collision is given by

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100 eV	0.76	3.53	4.57	4.062	3.64
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Table 3. The differential cross sections ($a_0^2 \text{Sr}^{-1}$) for the elastic scattering of positrons by helium atoms for energy 400 eV. The numbers in parentheses indicate powers of ten.

400 eV				
Energy (deg.)	Das <i>et al</i> (1981)	Modified Das method (Kusum Lata 1984)	EBS	Present UEBS
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60	1.03 (-2)	1.03 (-2)	1.16 (-2)	1.078 (-2)
70	6.52 (-3)	6.31 (-3)	7.82 (-3)	6.849 (-3)
80	4.45 (-3)	4.16 (-3)	5.66 (-3)	4.836 (-3)
90	3.24 (-3)	2.91 (-3)	4.34 (-3)	3.577 (-3)
100	2.49 (-3)	2.14 (-3)	3.48 (-3)	2.790 (-3)
120	1.67 (-3)	1.33 (-3)	2.49 (-3)	1.790 (-3)
140	1.28 (-3)	9.61 (-4)	1.99 (-3)	1.402 (-3)
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Das method (Das *et al* 1981), modified Das method (Kusum Lata 1984) and experimental results of Kauppila *et al* (1981). The experimental results of DCS for e^+ -He elastic collision are not available. At 100 eV, the present TCS value is greater than those of Das method, modified Das method and Kauppila *et al* (1981) by 81%, 13% and 10% respectively and less than that of EBS by 12%. At 400 eV, above percentage values are obtained 50%, 3%, 1% and 3% respectively. This shows that the difference between the present TCS value and those due to other methods decreases as the energy increases.

The present TCS results are greater than those of Kauppila *et al* (1981) by 10% and 1% at the energies 100 eV and 400 eV respectively while the TCS results of EBS method are greater than those of Kauppila *et al* (1981) by 20% and 4% at the energies 100 eV and 400 eV respectively. Thus the present TCS results yield better agreement with the experimental results than those due to EBS method. This indicates the improvement over EBS method due to unitarisation. The present DCS values are less than those of EBS and greater than those of Das method at all the given scattering angles and energies. The difference between the present DCS results and those of the other theoretical results is small at small angles and large at large angles. At particular angle the said difference decreases as the energy increases.

In the above comparison, the results of Das method are found in poor agreement with the present results and also with the other theoretical and experimental results. The reason for the above discrepancy has been discussed by the earlier workers which is represented here in brief. In Das method second Born term is multiplied by an energy dependent complex parameter to partially compensate for the missing higher Born terms. Jhanwar *et al* (1982c) have shown that in Das method the real parts of the forward scattering amplitude for electron hydrogen-collision and electron-helium collision are not even in qualitative agreement with the dispersion relation results of de Heer *et al* (1977). To improve Das method Khare and Lata (1984) introduced second Born term in the trial input scattering amplitude and considered the parameters not only energy dependent but also the function of scattering angle. With this modification in Das method Kusum Lata (1984) obtained better results which are taken here for comparison.

Byron *et al* (1982) calculated TCS for elastic scattering of positrons by hydrogen atom in intermediate energy region using UEBS method and found better agreement with the experimental results as compared with EBS results. Similarly the present UEBS results for e^+ -He elastic collision in intermediate energy region are found in better agreement with the experimental results as discussed above.

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